2,2,4-TRIMETHYLPENTANE

2,2,4-Trimethylpentane is a federal hazardous air pollutant and was identified as a toxic air contaminant in April 1993 under AB 2728.

CAS Registry Number: 540-84-1 $CH_3C(CH_3)_2CH_2CH(CH_3)CH_3$

Molecular Formula: C_8H_{18}

2,2,4-Trimethylpentane is a clear, mobile liquid with an odor of gasoline. It is highly flammable. It is practically insoluble in water and somewhat soluble in absolute alcohol (Merck, 1989). 2,2,4-Trimethylpentane is soluble in benzene, toluene, xylene, chloroform, ether, carbon disulfide, carbon tetrachloride, DMF, acetone, heptane, and oils (except castor oil) (HSDB, 1991).

Physical Properties of 2,2,4-Trimethylpentane

Synonyms: isobutyltrimethylethane; isooctane

Molecular Weight:	114.22
Boiling Point:	99.23 °C
Melting Point:	-107.45 °C
Flash Point:	10 °F (closed cup)
Vapor Density:	3.93 (air = 1)
Vapor Pressure:	40.6 mm Hg at 21 °C
Density/Specific Gravity:	0.69194 at 20/4 °C (water = 1)
Conversion Factor:	1 ppm = 4.67 mg/m^3

(HSDB, 1991; Merck, 1989; Sax, 1987; Sax, 1989; U.S. EPA, 1994a)

SOURCES AND EMISSIONS

A. Sources

2,2,4-Trimethylpentane is used as a standard reference fuel for octane ratings, since it has an antiknock octane number of 100. It is also used in spectrophotometric analysis, in organic synthesis, as an azeotropic distillation entrainer, and as a solvent and thinner (HSDB, 1991). The primary sources that have reported emissions of 2,2,4-trimethylpentane in California are public order and safety facilities, and gold and silver ores mining (ARB, 1997b).

2,2,4-Trimethylpentane has also been detected but not quantified in motor vehicle exhaust by the Air Resources Board (ARB) (ARB, 1995e).

B. Emissions

The total emissions of 2,2,4-trimethylpentane from stationary sources in California are estimated to be at least 4 pounds per year, based on data obtained from the Air Toxics "Hot Spots" Program (AB 2588) (ARB, 1997b).

C. Natural Occurrence

No information about the natural occurrence of 2,2,4-trimethylpentane was found in the readily-available literature.

AMBIENT CONCENTRATIONS

2,2,4-Trimethylpentane is monitored seasonally by the Air Resources Board at some sites in California that have elevated concentrations of ozone. The mean concentration of 2,2,4-trimethylpentane at four sites in 1993 is estimated to be 2.15 micrograms per cubic meter ($\mu g/m^3$) or 0.46 parts per billion (ppb) (ARB, 1995b).

The United States Environmental Protection Agency (U.S. EPA) has compiled ambient air data from 23 United States urban and suburban locations from 1971-86. An overall mean concentration of 22.5 $\mu g/m^3$ (4.82 ppb) was reported (U.S. EPA, 1993a).

INDOOR SOURCES AND CONCENTRATIONS

No information about the indoor sources of 2,2,4-trimethylpentane was found in the readily-available literature.

However, a study conducted in Raleigh, North Carolina measured 2,2,4-trimethylpentane inside vehicles. An average concentration of 17.0 $\mu g/m^3$ (3.6 ppb) and a maximum concentration of 95.3 $\mu g/m^3$ (20.4 ppb) was measured (Chan et al., 1991a).

ATMOSPHERIC PERSISTENCE

The dominant tropospheric loss process for 2,2,4-trimethylpentane is by reaction with the hydroxyl (OH) radical. The calculated half-life and lifetime of 2,2,4-trimethylpentane due to reaction with the OH radical are 2.8 days and 4.0 days, respectively (Atkinson, 1995). The reaction products of 2,2,4-trimethylpentane include aldehydes and ketones (Kao, 1994).

AB 2588 RISK ASSESSMENT INFORMATION

2,2,4-Trimethylpentane emissions are not reported from stationary sources in California under the AB 2588 program. It is also not listed in the California Air Pollution Control Officers Association Air Toxics "Hot Spots" Program Revised 1992 Risk Assessment Guidelines as having health values (cancer or non-cancer) for use in risk assessments (CAPCOA, 1993).

HEALTH EFFECTS

The most probable route of human exposure to 2,2,4-trimethylpentane is inhalation.

Non-Cancer: 2,2,4-Trimethylpentane is a respiratory tract irritant and central nervous system depressant. Little information is available on the acute effects of 2,2,4-trimethylpentane overexposure in humans. Rodents exposed by inhalation and injection developed lung irritation, edema, and hemorrhage. Acute inhalation exposure has been reported to cause central nervous system depression in mice (U.S. EPA, 1994a).

According to the U.S. EPA, no information is available on chronic effects of exposure to 2,2,4-trimethylpentane in humans. The U.S. EPA has not established a Reference Concentration (RfC) or an oral Reference Dose (RfD) for 2,2,4-trimethylpentane (U.S. EPA, 1994a).

No information on adverse reproductive effects in humans or animals is available (U.S. EPA, 1994a).

Cancer: No information is available on the carcinogenic potential of 2,2,4-trimethylpentane in humans or animals (U.S. EPA, 1994a). The International Agency for Research on Cancer and the U.S. EPA have not classified 2,2,4-trimethylpentane as to its potential carcinogenicity (IARC, 1987a; U.S. EPA, 1994a).